

Multiplicative Zagreb indices of cacti

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Abstract

Let $\prod(G)$ be Multiplicative Zagreb index of a graph G . A connected graph is a cactus graph if and only if any two of its cycles have at most one vertex in common, which has been the interest of researchers in the field of material chemistry and graph theory. In this paper, we use a new tool to obtain upper and lower bounds of $\prod(G)$ for all cactus graphs and characterize the corresponding extremal graphs.

Keywords: Extremal bounds; Multiplicative Zagreb index; Cactus graph.

AMS subject classification: 05C12, 05C05

1 Introduction

During recent decades, applied graph theory, molecular topology and mathematical chemistry have been the focus of considerable research in developed theory. In the field of chemical molecular graphs [9,14], the atoms are represented by vertices and the bonds by edges that capture the structural essence of compounds. The numerical representation of the molecule graph can be mathematically deduced as a single number, usually called graph invariant, molecular descriptor or topological index.

One of the oldest and most thoroughly considered molecular descriptor is Zagreb index which was introduced by Gutman and Trinajstić in 1972[6] as below: The first Zagreb index M_1 is the sum of the square vertex degrees of all the atoms and the second Zagreb index M_2 is the sum over all bonds of the product of the vertex degrees of the two adjacent atoms, that is, for any graph $G = (V, E)$ with vertex set $V(G)$ and edge set $E(G)$,

$$M_1(G) = \sum_{u \in V(G)} d(u)^2, M_2(G) = \sum_{uv \in E(G)} d(u)d(v).$$

In the 1980s, Narumi and Katayama [14] characterized the structural isomers of saturated hydrocarbons and considered the product $NK = \prod_{v \in V(G)} d(v)$, which is called the "Narumi-Katayama

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index". Recently, Todeschini et al.[5,7], Wang and Wei[16] studied the first (generalized) and second Multiplicative Zagreb indices defined as follows: For $c > 0$,

$$\prod_1(G) = \prod_{v \in V(G)} d(v)^c, \prod_2(G) = \prod_{uv \in E(G)} d(u)d(v).$$

Obviously, the first Multiplicative Zagreb index is the power of the NK index. Moreover, the second Multiplicative Zagreb index can be rewritten as $\prod_2(G) = \prod_{v \in V(G)} d(v)^{d(v)}$.

In the past several years, there are a lot of significant and interesting results [8,15] about chemical indices to the study of a computational complexity and the intersection between graph theory and chemistry. For general graphs, a lower bound of a chemical index, called Randić index, was given by Bollobas and Erds(1998)[1], while an upper bound was recently presented in (2004)[13]. In 2004, Das [2] applied the minimal and maximal degree to obtain the upper bound for the sum of the squares of the degrees of a graph, the first Zagreb index. In 2010, Zhao and Li [18] provided the maximal Zagreb index of graphs with k cut vertices. Estes and Wei (2014)[4], Wang and Wei (2015)[16] gave the sharp upper and lower bounds of Zagreb indices and Multiplicative Zagreb indices of k -trees, a generalization of a tree, respectively.

The synthetic resins[1], a type of plastic materials, is produced by the condensation of phenol with formaldehyde in the presence of a base. Independent benzene rings have no common edges in the diphenyl ether and the biphenyl. Many generic phenolic structures of clindamycin phosphate and cellulose have no shared edges between different phenolic molecules. Due to the properties, we consider a special class of graphs: A graph is a cactus if it is connected and all of its blocks are either edges or cycles, i.e., any two of its cycles have at most one common vertex. In 1969, Cornuéjols and Pulleyblank [3] used the constructure of a triangular cactus to find the equivalent conditions for the existence of $\{K_2, C_n, n \geq 4\}$ -factor. Also, Lin et al.(2007)[11], Liu and Lu (2008)[12] obtained some sharp bounds of several chemical indices of cactus graphs, such as Wiener index, Merrifield-Simmons index, Hosoya index and Randić index. In 2012, Li et al.[10] gave the upper bounds on Zagreb indices of cactus graphs and lower bounds of cactus graph with at least one cycle. Wang and Kang(2015) [17] found the extremal bounds of another chemical index, Harary index, for the cacti as well.

In this paper, we use the new tool of interesting functions to obtain sharp bounds of Multiplicative Zagreb indices on cacti, which can partially indicate the strength of heat resistance and flame retardancy by maximal and minimal bounds. By taking the derivatives, one can check the following facts.

Fact 1. *The function $f(x) = \frac{x}{x+m}$ is strictly increasing for $x \in [0, \infty)$, where m is a positive integer.*

Fact 2. *The function $f(x) = \frac{x^x}{(x+m)^{x+m}}$ is strictly decreasing for $x \in [0, \infty)$, where m is a positive integer.*

Since every cactus graph may have some pendant vertices which connect to one vertex only, then set C_n^k to denote a set of cactus graphs with n vertices including k pendant vertices, where

$n \geq k \geq 0$. An edge is called a pendant edge if one of its vertices is a pendant vertex. For $r \geq 1$, let $P_1 = u_1 u_2 \dots u_p v_1, P_2 = u_1 u_2 \dots u_p v_2, \dots, P_r = u_1 u_2 \dots u_p v_r$ be the paths of a graph G such that there exists at most one cycle C with $V(P_i) \cap V(C) = \{u_1\}$ and $d(v_i) = 1, i \geq 1$, then the induced subgraph $G[\{v_i, u_j, i \in [1, r], j \in [1, p]\}]$ is called a dense path. In particular, when $r = 1$, the dense path is a pendant path. The length of a dense path is the length of its pendant path. Theorems 1,2,3 provide sharp upper and lower bounds on the first generalized Multiplicative Zagreb indices of cactus graphs and characterize the extremal graphs.

Theorem 1 For any graph G in \mathcal{C}_n^k ,

$$\prod_{1,c}(G) \geq \begin{cases} 3^{kc} 2^{(n-2k)c} & \text{if } k = 0, 1, \\ 2^{(n-k-1)c} k^c & \text{if } k \geq 2, \end{cases}$$

the equalities hold if and only if their degree sequences are $\underbrace{3, 3, \dots, 3}_k, \underbrace{2, 2, \dots, 2}_{n-2k}, \underbrace{1, 1, \dots, 1}_k$ and $k, \underbrace{2, 2, \dots, 2}_{n-k-1}, \underbrace{1, 1, \dots, 1}_k$, respectively.

Theorem 2 For any graph G in \mathcal{C}_n^k with $n \leq k + 3$,

$$\prod_{1,c}(G) \leq \begin{cases} k^c & \text{if } n = k + 1, \\ (\lceil \frac{k}{2} \rceil + 1)^c (\lfloor \frac{k}{2} \rfloor + 1)^c & \text{if } n = k + 2, \\ (\lceil \frac{k}{3} \rceil + 2)^c (\lfloor \frac{k}{3} \rfloor + 2)^c (k - \lceil \frac{k}{3} \rceil - \lfloor \frac{k}{3} \rfloor + 2)^c & \text{if } n = k + 3, \end{cases}$$

the equalities hold if and only if their degree sequences are $k, \underbrace{1, 1, \dots, 1}_k; \lceil \frac{k}{2} \rceil + 1, \lfloor \frac{k}{2} \rfloor + 1, \underbrace{1, 1, \dots, 1}_k$ and $\lceil \frac{k}{3} \rceil + 2, \lfloor \frac{k}{3} \rfloor + 2, k - \lceil \frac{k}{3} \rceil - \lfloor \frac{k}{3} \rfloor + 2, \underbrace{1, 1, \dots, 1}_k$, respectively.

Theorem 3 For any graph G in \mathcal{C}_n^k with $n \geq k + 4$ and $t \geq 0$,

$$\prod_{1,c}(G) \leq \begin{cases} 16^c & \text{if } k = 0, n = 4, \\ 2^{(3t+6)c} & \text{if } k = 0, n = 2t + 5, \\ 2^{(3t+4)c} 9^c & \text{if } k = 0, n = 2(t + 3), \end{cases}$$

the equalities hold if and only if their degree sequences are $2, 2, 2, 2; \underbrace{4, 4, \dots, 4}_{t+1}, \underbrace{2, 2, \dots, 2}_{t+4}$ and $\underbrace{4, 4, \dots, 4}_t, 3, 3, \underbrace{2, 2, \dots, 2}_{t+4}$, respectively;

For $k \neq 0$, if $\prod_{1,c}(G)$ attains the maximal value, then one of the following statements holds: For any nonpendant vertices u, v , either (i) $|d(u) - d(v)| \leq 1$ or (ii) $d(u) \in \{2, 3, 4\}$ and G contains no cycles of length greater than 3, no dense paths of length greater than 1 except for at most one of them with length 2, no paths of length greater 0 that connects only two cycles except for at most one of them with length 1.

Theorems 4, 5 give the sharp upper and lower bounds on the second Multiplicative Zagreb indices of cactus graphs and characterize the extremal graphs.

Theorem 4 For any graph G in \mathcal{C}_n^k with $\gamma = \frac{k-2}{n-k}$,

$$\prod_2(G) \geq \begin{cases} 3^{3k} 2^{2(n-2k)} & \text{if } k = 0, 1, \\ (2 + \lceil \gamma \rceil)^{(2 + \lceil \gamma \rceil)[k-2 - \lfloor \gamma \rfloor(n-k)]} (2 + \lfloor \gamma \rfloor)^{(2 + \lfloor \gamma \rfloor)[n-2k+2 + \lfloor \gamma \rfloor(n-k)]} & \text{if } k \geq 2, \end{cases}$$

the equalities hold if and only if their degree sequences are $\underbrace{3, 3, \dots, 3}_k, \underbrace{2, 2, \dots, 2}_{n-2k}, \underbrace{1, 1, \dots, 1}_k$ and $\underbrace{2 + \lceil \gamma \rceil, 2 + \lceil \gamma \rceil, \dots, 2 + \lceil \gamma \rceil}_{k-2 - \lfloor \gamma \rfloor(n-k)}, \underbrace{2 + \lfloor \gamma \rfloor, 2 + \lfloor \gamma \rfloor, \dots, 2 + \lfloor \gamma \rfloor}_{n-2k+2 + \lfloor \gamma \rfloor(n-k)}, \underbrace{1, 1, \dots, 1}_k$, respectively.

Theorem 5 For any graph G in \mathcal{C}_n^k ,

$$\prod_2(G) \leq \begin{cases} (n-2)^{n-2} 2^{2(n-k-1)} & \text{if } n-k \equiv 0 \pmod{2}, \\ (n-1)^{n-1} 2^{2(n-k-1)} & \text{if } n-k \equiv 1 \pmod{2}, \end{cases}$$

the equalities hold if and only if their degree sequences are $n-2, \underbrace{2, 2, \dots, 2}_{n-k-1}, \underbrace{1, 1, \dots, 1}_k$ and $n-1, \underbrace{2, 2, \dots, 2}_{n-k-1}, \underbrace{1, 1, \dots, 1}_k$, respectively.

2 Preliminary

In this section, we will list some concepts and Lemmas which are critical in the late proofs.

As usual, $G = (V, E)$ is a simple connected graph and $|G|$ denotes the cardinality of V . For $S \subseteq V(G)$ and $F \subseteq E(G)$, $G[S]$ is the subgraph of G induced by S , $G - S$ is the subgraph induced by $V(G) - S$ and $G - F$ is the subgraph of G obtained by deleting F . Let $w(G - S)$ be the number of components of $G - S$ and S is a cut set if $w(G - S) \geq 2$. For a vertex $v \in V(G)$, the neighborhood of v is the set $N(v) = N_G(v) = \{w \in V(G), vw \in E(G)\}$, $d_G(v)$ or $d(v)$ is the degree of v with $d_G(v) = |N(v)|$. A tree T is called a pendant tree, if T has at most one vertex shared with some cycles in G . A biconnected graph is a connected graph having no cut vertices and a block is a maximal biconnected subgraph of a graph. In particular, the end block contains at most one cut vertex. Let $\lfloor x \rfloor$ be the largest integer that is less than or equal to x , $\lceil x \rceil$ be the smallest integer that is greater than or equal to x .

By the definition of Multiplicative Zagreb index, one can easily obtain the following lemmas.

Lemma 1 For $G \in \mathcal{C}_n^k$ with $k \leq 1$ and $n \geq 3$, if $\prod_{1,c}(G)$ or $\prod_2(G)$ attains the minimal value, then G is an unicyclic graph.

Proof. For $k = 0$ or 1 , by the choice of G , one can obtain that G contains at least one cycle. Otherwise, G is a tree which has at least two pendant vertices. Assume that there exists at least two cycles in G , and choose two cycles $C_1 = x_1 x_2 \dots x_1, C_2 = y_1 y_2 \dots y_1$ and a path $P = z_1 z_2 \dots z_p$ such that $V(P) \cap V(C_1) = \{z_1\}, V(P) \cap V(C_2) = \{z_p\}$ and P has no common vertices with any other cycles except C_1, C_2 . Let $N(z_1) \cap V(C_1) = \{x_{11}, x_{12}\}$ and $N(z_p) \cap V(C_1) = \{x_{p1}, x_{p2}\}$, and set $G' = (G - \{x_{11} z_1, x_{p1} z_p\}) \cup \{x_{11} x_{p1}\}$, then $d_{G'}(z_1) = d(z_1) - 1, d_{G'}(z_p) = d(z_p) - 1$. By the definitions

of $\Pi_{1,c}(G)$ and $\Pi_2(G)$, we have $\Pi_{1,c}(G') < \Pi_{1,c}(G)$ and $\Pi_2(G') < \Pi_2(G)$, a contradiction to the choice of G . Thus, Lemma 1 is true. \square

Lemma 2 *Let G' be a proper subgraph of a connected graph G , then $\Pi_{1,c}(G') < \Pi_{1,c}(G), \Pi_2(G') < \Pi_2(G)$. In particular, for $G \in \mathcal{C}_n^k$ with $k \geq 2$, if $\Pi_{1,c}(G)$ or $\Pi_2(G)$ attains the minimal value, then G is a tree.*

Proof. Since G' is a proper subgraph of G , by the definitions of $\Pi_{1,c}(G)$ and $\Pi_2(G)$, one can easily obtain that $\Pi_{1,c}(G') < \Pi_{1,c}(G)$ and $\Pi_2(G') < \Pi_2(G)$. For $k \geq 2$, we proceed to prove it by the contradiction. For $k \geq 2$, assume that G is not a tree, let C be a cycle of G and $P_1 = u_1 u_2 \dots u_p$ and $P_2 = v_1 v_2 \dots v_q$ be two pendant paths such that $V(P_1) \cap V(C) = \{u_1\}$ and $d(v_q) = 1$. Let $w_1 \in N(u_1) \cap V(C_1)$ and $G'' = (G - \{u_1 w_1, v_1 v_2\}) \cup \{v_2 w_1\}$, then $d_{G''}(u_1) = d(u_1) - 1, d_{G''}(v_1) = d(v_1) - 1$ and $G'' \in \mathcal{C}_n^k$. By the definitions of $\Pi_{1,c}(G)$ and $\Pi_2(G)$, we have $\Pi_{1,c}(G'') < \Pi_{1,c}(G), \Pi_2(G'') < \Pi_2(G)$ and Lemma 2 is true. \square

Lemma 3 *If $\Pi_2(G)$ attains the minimal value with $k \geq 2$, then any non-pendant vertices u, v of a connected graph G have the property: $|d(u) - d(v)| \leq 1$.*

Proof. Since $k \geq 2$, by Lemma 2, we have G must be a tree. On the contrary, if there are two non-pendant vertices $u, v \in V(G)$ such that $d(u) - d(v) \geq 2$, let $x \in N(u) - N(v)$ and $G' = (G - \{ux\}) \cup \{vx\}$, by Fact 2 and $d_{G'}(u) = d(u) - 1, d_{G'}(v) = d(v) + 1, d(v) \leq d(u) - 2 < d(u) - 1$, we have

$$\frac{\Pi_2(G)}{\Pi_2(G')} = \frac{d(v)^{d(v)} d(u)^{d(u)}}{[d(v) + 1]^{d(v)+1} [d(u) - 1]^{d(u)-1}} = \frac{\left[\frac{d(v)^{d(v)}}{[d(v)+1]^{d(v)+1}} \right]}{\left[\frac{[d(u)-1]^{d(u)-1}}{d(u)^{d(u)}} \right]} > 1,$$

that is, $\Pi_2(G') < \Pi_2(G)$, a contradiction with the choice of G . Thus, Lemma 3 is true. \square

Lemma 4 *If $\Pi_{1,c}(G)$ or $\Pi_2(G)$ attains the maximal value, then all cycles of G have length 3 except for at most one of them with length 4.*

Proof. On the contrary, let C_m be a cycle of G with $C_m = v_1 v_2 \dots v_m v_1$ and $m \geq 5$, $G' = (G - \{v_3 v_4\}) \cup \{v_1 v_3, v_1 v_4\}$. Since G' has k pendant vertices, then $G' \in \mathcal{C}_n^k$. By the definitions of $\Pi_{1,c}(G)$, $\Pi_2(G)$ and $d_{G'}(v_1) = d(v_1) + 2$, we have

$$\frac{\Pi_{1,c}(G)}{\Pi_{1,c}(G')} = \frac{d(v_1)^c}{[d(v_1) + 2]^c} < 1, \frac{\Pi_2(G)}{\Pi_2(G')} = \frac{d(v_1)^{d(v_1)}}{[d(v_1) + 2]^{d(v_1)+2}} < 1,$$

that is, $\Pi_{1,c}(G) < \Pi_{1,c}(G')$ and $\Pi_2(G) < \Pi_2(G')$, a contradiction with the choice of G . We can proceed this process until all of the cycles have length 3 or 4.

If there exist two cycles of length 4, say $C_1 = x_1 x_2 x_3 x_4 x_1, C_2 = y_1 y_2 y_3 y_4 y_1$ in G . Since G is a cactus, then there exists a vertex $x_t \in V(C_1)$ (say x_4) such that there are no paths connecting x_4 and y_1, x_4 and y_2 in $G - \{x_1 x_4, x_3 x_4\}$. Otherwise, if every vertex of $V(C)$ is either connected with y_1 or with y_2 in $G - \{x_1 x_4, x_3 x_4\}$, then there exist a cycle that shares at least one common edge with C_1 , a contradiction with the definition of cactus graph. Let $G^* = (G - \{x_1 x_4, x_3 x_4, y_1 y_4\}) \cup \{x_1 x_3, x_4 y_1, x_4 y_2, y_2 y_4\}$. Since G^* has k pendant vertices, then $G^* \in \mathcal{C}_n^k$. By the definitions of $\Pi_{1,c}(G)$,

$\Pi_2(G)$ and $d_{G^*}(y_2) = d(y_2) + 2$, we have

$$\frac{\Pi_{1,c}(G)}{\Pi_{1,c}(G^*)} = \frac{d(y_2)^c}{[d(y_2) + 2]^c} < 1, \frac{\Pi_2(G)}{\Pi_2(G^*)} = \frac{d(y_2)^{d(y_2)}}{[d(y_2) + 2]^{d(y_2)+2}} < 1,$$

that is, $\Pi_{1,c}(G) < \Pi_{1,c}(G^*)$ and $\Pi_2(G) < \Pi_2(G^*)$, a contradiction with the choice of G and Lemma 4 is true. \square

Lemma 5 *If $\Pi_{1,c}(G)$ or $\Pi_2(G)$ attains the maximal value, then every dense path has length 1 except for at most one of them with length 2.*

Proof. On the contrary, let C be a cycle and $P = v_1v_2\dots v_{p-1}v_{p_i}$ with $p \geq 2$ and $j \geq 1$ be a dense path such that $V(C) \cap V(P) = \{v_1\}$ and $d(v_{p_i}) = 1$. If $p \geq 4$, let $G' = G \cup \{v_1v_{p-1}\}$. Then $G' \in G[n, k]$ and $d_{G'}(v_1) = d(v_1) + 1$, $d_{G'}(v_{p-1}) = d(v_{p-1}) + 1$. Thus, by the definition, we have $\Pi_{1,c}(G') > \Pi_{1,c}(G)$ and $\Pi_2(G') > \Pi_2(G)$, a contradiction with the choice of G . We can proceed this process until $p \leq 3$, that is, all of the dense paths have the length as 1 or 2.

If there exist two such paths of length 2, say $P_1 = x_1x_2x_{3j}$, $P_2 = y_1y_2y_{3j'}$ with $x_1 \in V(C_2)$, $y_1 \in V(C_3)$ such that $d(x_{3j}) = d(y_{3j'}) = 1$ and $j, j' \geq 1$, then let $G^* = (G - \{y_1y_2, y_2y_{31}\}) \cup \{y_1y_{31}, x_1y_2, x_2y_2\}$. Since G^* has k pendant vertices, then $G^* \in G[n, k]$. By the definitions of $\Pi_{1,c}(G)$, $\Pi_2(G)$ and $d_{G^*}(x_1) = d(x_1) + 1$, $d_{G^*}(x_2) = d(x_2) + 1$, we have $\Pi_{1,c}(G^*) > \Pi_{1,c}(G)$ and $\Pi_2(G^*) > \Pi_2(G)$, a contradiction with the choice of G and Lemma 5 is true. \square

Lemma 6 *If $\Pi_{1,c}(G)$ or $\Pi_2(G)$ attains the maximal value, then G can not have both a dense path of length 2 and a cycle of length 4.*

Proof. On the contrary, let C_1 be a cycle, $P = y_1y_2y_{3i}$ be a dense path such that $V(C_1) \cap V(P) = \{y_1\}$ and $d(y_{3i}) = 1$ for $i \geq 1$, C_2 be a cycle of length 4, say $C_2 = x_1x_2x_3x_4x_1$. By the definition of the cactus, there exists $x_t \in V(C_2)$ (say x_2) such that there is no paths connecting x_2 and y_1 , x_2 and y_1 in $G - \{x_1x_2, x_2x_3\}$. Let $G' = (G - \{x_1x_2, x_2x_3\}) \cup \{x_2y_1, x_2y_2, x_1x_3\}$, then G' has k pendent vetices, $d_{G'}(y_1) = d(y_1) + 1$ and $d_{G'}(y_2) = d(y_2) + 1$. By the definitions of $\Pi_{1,c}(G)$, $\Pi_2(G)$, we have $\Pi_{1,c}(G') > \Pi_{1,c}(G)$ and $\Pi_2(G') > \Pi_2(G)$, a contradiction with the choice of G and Lemma 6 is true. \square

Lemma 7 *Let C be a cycle of G in \mathcal{C}_n^k and $u, v \in V(C)$, if $\min\{d(u), d(v)\} > 2$, then there exist a graph G' such that $\Pi_2(G') > \Pi_2(G)$.*

Proof. Since $\min\{d(u), d(v)\} \geq 3$, without loss of generality, let $d(u) \geq d(v) \geq 3$, then there exist $x \in N(v) - V(C) - N(u)$, otherwise, there will be two cycles containing at least two common vertices. Let $G' = (G - \{vx\}) \cup \{ux\}$, we have $d(u) \geq d(v) > d(v) - 1$. By Fact 2, we have

$$\frac{\Pi_2(G)}{\Pi_2(G')} = \frac{d(u)^{d(u)}d(v)^{d(v)}}{[d(u) + 1]^{d(u)+1}[d(v) - 1]^{d(v)-1}} = \frac{\frac{d(u)^{d(u)}}{[d(u)+1]^{d(u)+1}}}{\frac{[d(v)-1]^{d(v)-1}}{d(v)^{d(v)}}} < 1.$$

Thus, $\Pi_2(G') > \Pi_2(G)$ and Lemma 7 is true. \square

Lemma 8 *If $\Pi_2(G)$ attains the maximal value, then any three cycles have a common vertex.*

Proof. By the definition of the cactus, any two cycles have at most one common vertex. Now assume that there exist two disjoint cycles C_1, C_2 contained in G such that the path P connecting C_1 and C_2 is as short as possible. For convenience, let $P = u_1 u_2 \dots u_p$, $V(P) \cap V(C_1) = \{u_1\}$ and $V(P) \cap V(C_2) = \{u_p\}$.

If the path P has no common edges with any other cycle(s) contained in G and $|E(P)| \geq 2$, let the new graph $G' = G \cup \{u_1 u_p\}$, then $G' \in G[n, k]$, $d_{G'}(u_1) = d(u_1) + 1$, $d_{G'}(u_p) = d(u_p) + 1$. By the definition of $\Pi_2(G)$, we have $\Pi_2(G') > \Pi_2(G)$. If $|E(P)| = 1$, without loss of generality, let $d(u_1) \geq d(u_2)$ and $C_2 = u_2 v_2 v_3 \dots u_2$, we have $v_2 \notin N(u_1)$. Otherwise, there are two cycles who have the common edge contradicted with the definition of the cactus. Let $G^* = (G - \{u_2 v_2\}) \cup \{u_1 v_2\}$, we have $G^* \in G[n, k]$, $d_{G^*}(u_1) = d(u_1) + 1$ and $d_{G^*}(u_2) = d(u_2) - 1$. Since $d(u_1) \geq d(u_2) > d(u_2) - 1$, then

$$\frac{\Pi_2(G)}{\Pi_2(G^*)} = \frac{d(u_1)^{d(u_1)} d(u_2)^{d(u_2)}}{[d(u_1) + 1]^{d(u_1)+1} [d(u_2) - 1]^{d(u_2)-1}} = \frac{\left[\frac{d(u_1)^{d(u_1)}}{[d(u_1)+1]^{d(u_1)+1}} \right]}{\left[\frac{[d(u_2)-1]^{d(u_2)-1}}{d(u_2)^{d(u_2)}} \right]} < 1,$$

that is, $\Pi_2(G^*) > \Pi_2(G)$, a contradiction with the choice of G .

If P has some common edges with some other cycle, say C_3 , by the choice of C_1, C_2 and the definitions of cactus graph, we have $\{u_1\} = C_3 \cap C_1$ and $\{u_p\} = C_3 \cap C_2$. Since $\min\{d(u_1), d(u_p)\} \geq 3$, by Lemma 7, we can get that there exist G^{**} such that $\Pi_2(G^{**}) > \Pi_2(G)$, a contradiction with the choice of G .

Thus, any two cycles of G have one common vertex. By the definition of cactus graph, we have that any three cycles have exactly one common vertex and Lemma 8 is true. \square

Lemma 9 *Let T be a tree attached to a vertex v_0 of a cycle of G , if $\Pi_2(G)$ attains the maximal value, then $d(v) \leq 2$ for any $v \in V(T) - \{v_0\}$.*

Proof. Choose a graph G such that $\Pi_2(G)$ achieves the maximal value. On the contrary, assume that $u \in V(T) - \{v_0\}$ is of degree $r \geq 3$ and closest to a pendant vertex. For $d(u, v_0) \geq 2$, let $G' = G \cup \{uv_0\}$, we have $G' \in G[n, k]$, $d_{G'}(u) = d(u) + 1$ and $d_{G'}(v_0) = d(v_0) + 1$. By the definition of $\Pi_2(G)$, we can obtain that $\Pi_2(G') > \Pi_2(G)$, a contradiction with the choice of G . For $d(u, v_0) = 1$, let $\{y_1, y_2, \dots, y_{r-2}\}$ be the $r-2$ neighbors of u such that $d(y_i, v_0) > d(u, v_0)$, y be a neighbor of v_0 which belongs to a cycle C_0 .

Since $v_0 u y_1$ is a pendant path of length 2, by Lemma 6, we have that every cycle has length 3. Let $C_0 = v_0 w_1 y v_0$, $G'' = (G - \{u y_1\}) \cup \{v_0 y_1\}$ and $G''' = (G - \{v_0 y\}) \cup \{u y\}$, then $G'', G''' \in G[n, k]$, $d_{G''}(u) = d(u) - 1$, $d_{G''}(v_0) = d(v_0) + 1$ and $d_{G'''}(u) = d(u) + 1$, $d_{G'''}(v_0) = d(v_0) - 1$. By the definition of $\Pi_2(G)$ and Fact 2, we can obtain

$$\frac{\Pi_2(G)}{\Pi_2(G'')} = \frac{d(u)^{d(u)} d(v_0)^{d(v_0)}}{[d(u) - 1]^{d(u)-1} [d(v_0) + 1]^{d(v_0)+1}} = \frac{\left[\frac{d(v_0)^{d(v_0)}}{[d(v_0)+1]^{d(v_0)+1}} \right]}{\left[\frac{[d(u)-1]^{d(u)-1}}{d(u)^{d(u)}} \right]} < 1, \text{ if } d(v_0) \geq d(u),$$

$$\frac{\Pi_2(G)}{\Pi_2(G''')} = \frac{d(u)^{d(u)} d(v_0)^{d(v_0)}}{[d(u) + 1]^{d(u)+1} [d(v_0) - 1]^{d(v_0)-1}} = \frac{\left[\frac{d(u)^{d(u)}}{[d(u)+1]^{d(u)+1}} \right]}{\left[\frac{[d(v_0)-1]^{d(v_0)-1}}{d(v_0)^{d(v_0)}} \right]} < 1, \text{ if } d(v_0) < d(u),$$

that is, $\Pi_2(G'') > \Pi_2(G)$ and $\Pi_2(G''') > \Pi_2(G)$, a contradiction with the choice of G . Thus, Lemma 9 is true. \square

Lemma 10 *If $\Pi_2(G)$ attains the maximal value, then all attached trees are attached to a common vertex v_0 .*

Proof. On the contrary, suppose that there exist two trees T_1, T_2 attached to different vertices v_1, v_2 of some cycles, say C_1, C_2 , such that $V(C_1) \cap V(T_1) = \{v_1\}, V(C_2) \cap V(T_2) = \{v_2\}$. By Lemma 8, all the cycles have a common vertex v_0 . Without loss of generality, let $v_1 \neq v_0$, we have $d(v_0) \geq 3, d(v_1) \geq 3$. By Lemma 7, there exists G' such that $\Pi_2(G') > \Pi_2(G)$, a contradiction to the choice of G . Thus, Lemma 10 is true. \square

3 Main proofs

In this section, we will prove the main results. For any graph G in \mathcal{C}_n^k , if $n = 1$ or 2 , then $\Pi_{1,c}(G) = \Pi_2(G) = 0$ or 1 , that is, all upper and lower bounds of Multiplicative Zagreb indices have the same values, respectively. Thus, all of the Theorems are true. Now we may assume that $n \geq 3$.

Proof of Theorem 1. Choose a graph G in \mathcal{C}_n^k such that $\Pi_{1,c}(G)$ achieves the minimal value. For $k \leq 1$, by Lemma 1, G is an unicyclic graph. If $k = 0$, then G is a cycle, that is, the degree sequence of G is $\underbrace{2, 2, \dots, 2}_n$; If $k = 1$, then G has only one pendant path, that is, the degree sequence of G is $\underbrace{3, 2, 2, \dots, 2}_{n-2}, 1$. Thus, Theorem 1 is true.

For $k \geq 2$, by the choice of G and Lemma 2, we obtain that G is a tree. If $k = 2$, then G is a path, that is, the degree sequence of G is $\underbrace{2, 2, \dots, 2}_{n-2}, 1, 1$ and Theorem 1 is true; For $k \geq 3$, if there is a vertex v with $d(v) \geq k + 1$, since G is a tree, then G has more than k pendant vertices, a contradiction to the choice of G . Thus, $d(v) \leq k$ for any $v \in V(G)$. Now let v be the vertex with maximal degree Δ , if $\Delta = k$, then $G - v$ is a set of paths. Otherwise, there exists a vertex $u \in V(G) - \{v\}$ such that $d(u) \geq 3$ and since G is a tree, then G contains more than k pendant vertices, a contradiction to the choice of G . Thus, the degree sequence of G is $\underbrace{k, 2, 2, \dots, 2}_{n-k-1}, \underbrace{1, 1, \dots, 1}_k$.

If $\Delta < k$, then G contains at least 2 cut vertices, say u_1, u_2, \dots, u_t , such that $G - u_i$ has at least 3 components with $i \in [1, t]$ and $t \geq 2$. Otherwise, since G is a tree, G only contains Δ pendant vertices. Let $P = w_1 w_2 \dots w_s$ be a path of $G - \{u_1, u_2, \dots, u_t\}$ such that $w_s \in \{u_1, u_2, \dots, u_t\} - \{v\}$ and P contains only a unique pendant vertex w_1 . Set $G' = (G - \{w_{s-1} w_s\}) \cup \{w_{s-1} v\}$, we have $G' \in \mathcal{C}_n^k$, $d_{G'}(v) = d(v) + 1$ and $d_{G'}(w_s) = d(w_s) - 1$. Thus, by $\Delta \geq d(w_s) > d(w_s) - 1$, we have

$$\frac{\Pi_{1,c}(G)}{\Pi_{1,c}(G')} = \frac{\Delta^c d(w_s)^c}{(\Delta + 1)^c (d(w_s) - 1)^c} = \frac{\frac{\Delta^c}{(\Delta + 1)^c}}{\frac{[d(w_s) - 1]^c}{d(w_s)^c}} > 1,$$

that is, $\Pi_{1,c}(G)$ is not minimal, a contradiction with the choice of G . If the maximal degree of G' is still less than k , then we can continue this process until $\Delta = k$, thus we can find the desired graph

with the degree sequence of $k, \underbrace{2, 2, \dots, 2}_{n-k-1}, \underbrace{1, 1, \dots, 1}_k$. Therefore, Theorem 1 is true. \square

Proof of Theorem 2. Choose a graph G in \mathcal{C}_n^k such that $\prod_{1,c}(G)$ achieves the maximal value. Let $S = \{v \in V(G), d(v) = 1\}$ and $G' = G - S$. If $|G'| = 1$, then for $k = 0$, the degree sequence of G is 0 and for $k \neq 0$, G is a star, that is, its degree sequence is $k, \underbrace{1, 1, \dots, 1}_k$. If $|G'| = 2$ and for $k = 0$, there is no such simple connected graph; For $k \neq 0$, by "Arithmetic-Mean and Geometric-Mean inequality: $x_1 x_2 \dots x_n \leq (\frac{x_1 + x_2 + \dots + x_n}{n})^n$, the equality holds if and only if $x_1 = x_2 = \dots = x_n$ ", one can obtain that the degree sequence of G is $\lceil \frac{k}{2} \rceil + 1, \lfloor \frac{k}{2} \rfloor + 1, \underbrace{1, 1, \dots, 1}_k$. If $|G'| = 3$ and $k = 0$, by Lemma 2, we can obtain that G is a cycle of length 3, that is, its degree sequence is 2, 2, 2. For $k \neq 0$, it is similar to the above proof, that is, the degree sequence of G is $\lceil \frac{k}{3} \rceil + 2, \lfloor \frac{k}{3} \rfloor + 2, k - \lceil \frac{k}{3} \rceil - \lfloor \frac{k}{3} \rfloor + 2, \underbrace{1, \dots, 1}_k$. Therefore, Theorem 2 is true. \square

Proof of Theorem 3. Choose a graph G in \mathcal{C}_n^k such that $\prod_{1,c}(G)$ achieves the maximal value. By Lemma 2 and $n - k \geq 4$, G contains some cycles. For $n - k = 4$, $G - S$ contains only one cycle C_0 , where $S = \{v \in V(G), d(v) = 1\}$. If $k = 0$, by the choice of G , one can obtain that G is a cycle, that is, its degree sequence is 2, 2, 2, 2. If $k \neq 0$ and $|C_0| = 4$, by adding any deleted vertex back to $G - S$, one can get a new graph G_{01} with degree sequence 3, 2, 2, 2, 1; If $k \neq 0$ and $|C_0| = 3$, by adding back any deleted vertex to $G - S$ such that it is adjacent to the pendant vertex in $G - S$, one can obtain a new graph G'_{01} . Since G_{01} and G'_{01} have the same degree sequences, by *Arithmetic-Mean and Geometric-Mean inequality*, we can continue to add any deleted vertex back to G_{01} or G'_{01} such that it is adjacent to the nonpendant vertex of smallest degree in G_{01} or G'_{01} . After adding back all of the deleted vertices, we can obtain the graph of maximal $\prod_{1,c}$ -value and Theorem 3 is true. Thus we will consider the case when $n - k \geq 5$ below. By the choice of G and Lemma 4, G contains at least two cycles.

Claim 1. *The longest path connecting only two cycles has length at most 1.*

Proof. On the contrary, let $C_l, C_{l'}$ be two cycles and $P_1 = x_1 x_2 \dots x_p$ be a path such that $V(C_l) \cap V(P_1) = \{x_1\}$, $V(C_{l'}) \cap V(P_1) = \{x_p\}$. If $p \geq 3$, set $G' = G \cup \{x_1 x_p\}$, then $d_{G'}(x_1) = d(x_1) + 1$ and $d_{G'}(x_p) = d(x_p) + 1$. By the definition of $\prod_{1,c}(G)$, we have $\prod_{1,c}(G') > \prod_{1,c}(G)$, a contradiction to the choice of G . Thus, $p \leq 2$ and Claim 1 is true. \square

We first deal with the case when $k = 0$.

Claim 2. *Any three cycles have no common vertex if $k = 0$.*

Proof. On the contrary, let C_1, C_2, C_3 be the cycles of G such that $\cap_{i=1}^3 V(C_i) = \{v_0\}$, and $N(v_0) \cap V(C_i) = \{v_{i1}, v_{i2}\}$ for $i \in [1, 3]$. Choose v of degree 2 such that v is in an end block C_t of G and $N(v) \cap V(C_t) = \{v_{t1}, v_{t2}\}$. Set $G'' = (G - \{v_{21}v_0, v_{22}v_0\}) \cup \{v_{21}v, v_{22}v\}$, then $d_{G''}(v_0) = d(v_0) - 2$ and $d_{G''}(v) = d(v) + 2$. Since $d(v_0) - 2 \geq 4 > d(v)$, By the definitions of $\prod_{1,c}(G)$ and Fact 1, we have

$$\frac{\prod_{1,c}(G)}{\prod_{1,c}(G'')} = \frac{d(v_0)^c d(v)^c}{[d(v_0) - 2]^c [d(v) + 2]^c} = \frac{\lceil \frac{d(v)^c}{[d(v)+2]^c} \rceil}{\lceil \frac{[d(v_0)-2]^c}{d(v_0)^c} \rceil} < 1,$$

that is, $\Pi_{1,c}(G'') > \Pi_1(G)$, a contradiction to the choice of G . \square

Claim 3. *Every vertex of G has the degree 2, 3 or 4 if $k = 0$.*

Proof. We will prove it by the contradiction. If there is a vertex w_1 with $d(w_1) \geq 5$, by Claim 2, we can assume that there are two cycles $C_4, C_{4'}$ and a path P_2 such that $V(C_4) \cap V(C_{4'}) \cap V(P_2) = \{w_1\}$, since $k = 0$ and G is a cactus, there exists a vertex w_0 of an end block such that $d(w_0) = 2$, that is, $d(w_0) < d(w_1) - 2$. Without loss of generality, assume that w_0 is closer to $C_{4'}$, let $N(w_1) \cap V(C_4) = \{w_2, w_3\}$ and $G''' = (G - \{w_1w_2, w_1w_3\}) \cup \{w_0w_2, w_0w_3\}$, by the definition of $\Pi_{1,c}(G)$ and Fact 1, we have

$$\frac{\Pi_{1,c}(G)}{\Pi_{1,c}(G''')} = \frac{d(w_1)^c d(w_0)^c}{[d(w_1) - 2]^c [d(w_0) + 2]^c} = \frac{\left\lceil \frac{d(w_0)^c}{[d(w_0) + 2]^c} \right\rceil}{\left\lceil \frac{d(w_1) - 2]^c}{d(w_1)^c} \right\rceil} < 1,$$

that is, $\Pi_{1,c}(G''') > \Pi_{1,c}(G)$, a contradiction to the choice of G . Thus, Claim 3 is true. \square

Claim 4. *There do not exist two paths of length 1 such that every path connects with only two cycles if $k = 0$.*

Proof. On the contrary, assume that there are two such paths $P_5 = z_1z_2$, $P_6 = y_1y_2$ with $z_1 \in C_6, z_2 \in C_7, y_1 \in C_8, y_2 \in C_9$ such that $N(y_1) \cap V(C_8) = \{y_{11}, y_{12}\}$ and $d(z_1) = d(z_2) = d(y_1) = d(y_2) = 3$. Let $G^* = (G - \{y_1y_2, y_1y_{11}, y_1y_{12}\}) \cup \{y_2y_{11}, y_2y_{12}, z_1y_1, z_2y_1\}$. Since $d_{G^*}(z_1) = d_{G^*}(z_2) = d_{G^*}(y_2) = 4, d_{G^*}(y_1) = 2$. By the definition of $\Pi_{1,c}(G)$ and Fact 1, we have

$$\frac{\Pi_{1,c}(G)}{\Pi_{1,c}(G^*)} = \frac{d(z_1)^c d(z_2)^c d(y_1)^c d(y_2)^c}{[d(z_1) + 1]^c [d(z_2) + 1]^c [d(y_1) - 1]^c [d(y_2) + 1]^c} = \frac{3^c 3^c 3^c 3^c}{4^c 4^c 2^c 4^c} < 1,$$

that is, $\Pi_{1,c}(G^*) > \Pi_{1,c}(G)$, a contradiction to the choice of G and Claim 4 is true. \square

Claim 5 *G can not have both a cycle of length 4 and a path of length 1 connecting only with two cycles if $k = 0$.*

Proof. On the contrary, let C_{10}, C_{11}, C_{12} be the cycles and $P = w_1w_2$ be a path such that $V(C_{10}) \cap V(P) = \{w_1\}$, $V(C_{11}) \cap V(P) = \{w_2\}$. If $|C_{10}| = |C_{11}| = 3$ and $|C_{12}| = 4$, then there exists a vertex $w_3 \in V(C_{12})$ such that $d(w_3) = 3$ or 4. Let $C_{12} = w_3x_2x_3x_4w_3$ and $G^{**} = (G - \{w_1w_2, x_2x_3\}) \cup \{w_2w_3, w_2x_2, w_3x_3\}$, then $d_{G^{**}}(w_1) = d(w_1) - 1 = 2, d_{G^{**}}(w_2) = d(w_2) + 1 = 4, d_{G^{**}}(w_3) = d(w_3) + 2 = 5$ or 6 and G^{**} has no pendent vetices. By the definitions of $\Pi_{1,c}(G)$, we have

$$\frac{\Pi_{1,c}(G)}{\Pi_{1,c}(G^{**})} = \frac{d(w_1)^c d(w_2)^c d(w_3)^c}{[d(w_1) - 1]^c [d(w_2) + 1]^c [d(w_3) + 2]^c} = \frac{3^c 3^c 3^c}{2^c 4^c 5^c} \text{ or } \frac{3^c 3^c 4^c}{2^c 4^c 6^c} < 1,$$

that is, $\Pi_{1,c}(G^{**}) > \Pi_{1,c}(G)$, a contradiction with the choice of G .

If $|C_{10}| = |w_1w_{12}w_{13}w_{14}w_1| = 4$ and $|C_{11}| = |w_2w_{22}w_{23}w_2| = 3$, then $d(w_1) = d(w_2) = 3, d(w_{14}) = 2$ or 4. Let $G^{***} = (G - \{w_1w_{12}\}) \cup \{w_{12}w_{14}, w_2w_{14}\}$, we have $G^{***} \in \mathcal{C}_n^k$, $d_{G^{***}}(w_1) = d(w_1) - 1, d_{G^{***}}(w_{14}) = d(w_{14}) + 2, d_{G^{***}}(w_2) = d(w_2) + 1$. By the definitions of $\Pi_{1,c}(G)$, we have

$$\frac{\Pi_{1,c}(G)}{\Pi_{1,c}(G^{***})} = \frac{d(w_1)^c d(w_{14})^c d(w_2)^c}{[d(w_1) - 1]^c [d(w_{14}) + 2]^c [d(w_2) + 1]^c} = \frac{3^c 2^c 3^c}{2^c 4^c 4^c} \text{ or } \frac{3^c 4^c 3^c}{2^c 6^c 4^c} < 1.$$

that is, $\Pi_{1,c}(G^{***}) > \Pi_{1,c}(G)$, a contradiction with the choice of G and Claim 5 is true. \square

Thus, for $k = 0$ and $n = 5$, by the choice of G and Lemma 4, there exist two cycles of length 3, that is, its degree sequence is $4, 2, 2, 2, 2$; For $n = 6$, G can be G_l or G_s such that G_l contains two cycles of length 3 or G_s contains one cycle of length 3 and one cycle of length 4, that is, the degree sequences are $3, 3, 2, 2, 2, 2$ and $4, 2, 2, 2, 2, 2$. Since $\prod_{1,c}(G_l) > \prod_{1,c}(G_s)$, then $\prod_{1,c}(G_l)$ attains the maximal value; Similarly, for $n \geq 7$, if $n = 2t + 5$ with $t \geq 1$, then G^a contains only the cycles of length 3 and its degree sequence is $\underbrace{4, 4, \dots, 4}_{t+1}, \underbrace{2, 2, \dots, 2}_{t+4}$; If $n = 2(t + 3)$, then G^b contains some cycles of length 3 and one path of length 1 that connects only two cycles, that is, its degree sequence is $\underbrace{4, 4, \dots, 4}_t, \underbrace{3, 3, 2, 2, \dots, 2}_{t+4}$.

Now we consider the case when $k \neq 0$ and define the following algorithm, say *Pro* : Step 1. Build G_{T_0} by deleting all the dense paths such that G_{T_0} satisfies the case of $k = 0$, that is, G_{T_0} is either G^a or G^b ; Step 2. Build G_{T_i} by adding a deleted path to $G_{T_{i-1}}$ such that it is adjacent to a non-pendant vertex of smallest degree in $G_{T_{i-1}}$, $i \geq 1$; Step 3. Stop, if there is no remaining deleted paths; Go to Step 2, if otherwise.

By the choice of G and Lemma 5, all of the dense paths of G have length 1 except for at most one of them with length 2. If all of the dense paths of G have length 1, by *Arithmetic-Mean and Geometric-Mean inequality*, we can directly use *Pro* to get a new graph G_T of maximal $\prod_{1,c}$ -value. Thus, for $k < 4 + t$, G_T contains no cycles of length greater than 3, no dense paths of length greater than 1, no paths of length greater 0 that connects only two cycles except for at most one of them with length 1 and $d_{G_T}(w_a) \in \{2, 3, 4\}$, where w_a is any nonpendant vertex of G_T ; For $k \geq 4 + t$, we have $|d_{G_T}(w_b) - d_{G_T}(w_c)| \leq 1$, where w_b, w_c are any nonpendant vertices of G_T , that is, the statement (i) or (ii) is true. If there is one of the dense paths of G with length 2, then set $P_1 = u_1 u_2 u_{31}$, $P_2 = u_1 u_2 u_{32}, \dots, P_{r-1} = u_1 u_2 u_{3(r-1)}$ with $d(u_{3i}) = 1, i \in [1, r-1]$. By *Arithmetic-Mean and Geometric-Mean inequality*, we can use *Pro* to get a new graph G_T such that $\prod_{1,c}(G_T) \geq \prod_{1,c}(G)$.

By the proof of the case for $k = 0$, if G_T contains a path $P_T = w_{T1} w_{T2}$ connecting only two cycles, say C_{T1}, C_{T2} , such that $V(C_{T1}) \cap V(P_T) = \{w_{T1}\}, V(C_{T2}) \cap V(P_T) = \{w_{T2}\}$, then set $G_1 = (G_T - \{u_2 u_i, i \in [1, r-1]\}) \cup \{u_{31} w_{T1}, u_{31} w_{T2}, u_{31} u_j, i \in [2, r-1]\}$. Since $G_1 \in \mathcal{C}_n^k$, $d_{G_1}(w_{T1}) = d(w_{T1}) + 1, d_{G_1}(w_{T2}) = d(w_{T2}) + 1, d(u_2) = r, d_{G_1}(u_2) = 1, d(u_{31}) = 1$ and $d_{G_1}(u_{31}) = r$, by the definition of $\prod_{1,c}(G)$ and Fact 1, we have

$$\frac{\prod_{1,c}(G)}{\prod_{1,c}(G_1)} = \frac{d(w_{T1})^c d(w_{T2})^c d(u_{31})^c d(u_2)}{[d(w_{T1}) + 1]^c [d(w_{T2}) + 1]^c d(u_{31})^c d_1(u_2)} < 1,$$

that is, $\prod_{1,c}(G_1) > \prod_{1,c}(G)$, a contradiction to the choice of G .

If G_T contains no such path P_T and $|d(u_2) - d(v_T)| \leq 1$ for any nonpendant vertices v_T, v'_T of G_T , when $|d(v_T) - d(v'_T)| \leq 1$, then the statement (i) is true; When there exist v_T, v'_T such that $|d(v_T) - d(v'_T)| > 1$, by the construction of G_T , we have $d(v_T), d(v'_T) \in \{2, 3, 4\}$ and G contains no dense paths of length greater than 1 except for at most one of them with length 2, that is, the statement (ii) is true. Otherwise, if there exists a vertex v_T such that $|d(u_2) - d(v_T)| > 1$, then without loss of generality, choose C_{T3} and C_{T4} such that $V(C_{T3}) \cap V(C_{T4}) = \{v_T\}$ and let

$N(v_T) = \{v_{ci}, i \geq 4\}$ such that $v_{c1}, v_{c2} \in V(C_{T3})$, $v_{c3}, v_{c4} \in V(C_{T3})$. When $d(v_T) - d(u_2) > 1$, set $G_2 = (G_T - \{v_T v_{c1}, v_T v_{c2}, u_2 u_{3i}, i \geq 1\}) \cup \{u_{31} v_{c1}, u_{31} v_{c2}, u_{31} v_T, u_{31} u_{3i}, i \geq 2\}$, then $d_{G_2}(u_2) = 1, d_{G_2}(u_{31}) = d(u_2) + 1$ and $d_{G_2}(v_T) = d(v_T) - 1$. When $d(u_2) - d(v_T) > 1$, that is, $d(u_2) > 3$, set $G_3 = (G_T - \{v_T v_{c1}, v_T v_{c2}, u_2 u_{3i}, i \geq 1\}) \cup \{u_{31} v_{c1}, u_{31} v_{c2}, u_{31} v_T, u_{32} v_T, u_{33} v_T, u_{31} u_{3i}, i \geq 4\}$, then $d_{G_3}(u_2) = 1, d_{G_3}(u_{31}) = d(u_2) - 1$ and $d_{G_3}(v_T) = d(v_T) + 1$. Since $G_2, G_3 \in \mathcal{C}_n^k$, by the definition of $\Pi_{1,c}(G)$ and Fact 1, we have

$$\frac{\Pi_{1,c}(G)}{\Pi_{1,c}(G_2)} = \frac{d(u_{31})^c d(u_2)^c d(v_T)^c}{[d(u_2) + 1]^c 1^c [d(v_T) - 1]^c} < 1, \frac{\Pi_{1,c}(G)}{\Pi_{1,c}(G_3)} = \frac{d(u_{31})^c d(u_2)^c d(v_T)^c}{[d(u_2) - 1]^c 1^c [d(v_T) + 1]^c} < 1,$$

that is, $\Pi_{1,c}(G_2) > \Pi_{1,c}(G)$, $\Pi_{1,c}(G_3) > \Pi_{1,c}(G)$, a contradiction to the choice of G . Therefore, Theorem 3 is true. \square

Proof of Theorem 4. Choose a graph G in \mathcal{C}_n^k such that $\Pi_2(G)$ achieves the minimal value. By Lemma 1, G is an unicyclic graph for $k \leq 1$. If $k = 0$, then G is a cycle, that is, its degree sequence is $\underbrace{2, 2, \dots, 2}_n$; If $k = 1$, then G has only one pendant path, that is, its degree sequence is $3, \underbrace{2, 2, \dots, 2}_{n-2}, 1$.

For $k \geq 2$, by Lemma 2, we only need to consider G as a tree. Since $\sum_{v \in V(G)} d(v) = 2(n-1)$, then the average degree of G except the pendant vertices is $\frac{\sum_{v \in V(G)} d(v) - k}{n-k} = \frac{2(n-1)-k}{n-k} = 2 + \frac{k-2}{n-k} = 2 + \gamma$. By Lemma 3, if all of nonpendant vertices have degree $2 + \lfloor \gamma \rfloor$ or $2 + \lceil \gamma \rceil$, then $\Pi_2(G)$ attains the minimal value. Set the number of the vertices with degree $2 + \lfloor \gamma \rfloor$ to be y_1 , the number of the vertices with degree $2 + \lceil \gamma \rceil$ to be y_2 , we have $y_1 + y_2 + k = n$ and $(2 + \lfloor \gamma \rfloor)y_1 + (2 + \lceil \gamma \rceil)y_2 + k = 2(n-1)$. If $\lfloor \gamma \rfloor = \lceil \gamma \rceil$, then Theorem 4 is true; If $\lceil \gamma \rceil - \lfloor \gamma \rfloor = 1$, by solving the above equations, we have $y_1 = n - 2k + 2 + \lfloor \gamma \rfloor(n-k), y_2 = k - 2 - \lfloor \gamma \rfloor(n-k)$, that is, its degree sequence is $\underbrace{2 + \lceil \gamma \rceil, 2 + \lceil \gamma \rceil, \dots, 2 + \lceil \gamma \rceil}_{k-2-\lfloor \gamma \rfloor(n-k)}, \underbrace{2 + \lfloor \gamma \rfloor, 2 + \lfloor \gamma \rfloor, \dots, 2 + \lfloor \gamma \rfloor}_{n-2k+2+\lfloor \gamma \rfloor(n-k)}, \underbrace{1, 1, \dots, 1}_k$. Therefore, Theorem 4 is true. \square

Proof of Theorem 5. Choose G in \mathcal{C}_n^k such that $\Pi_2(G)$ achieves the maximal value. By Lemma 4, the lengths of all cycles in G are 3 except for at most one of them with length 4; By Lemmas 5 and 9, every pendant path has length of 1 except for at most one of them with length 2. By Lemma 6, G can not have both a dense path of length 2 and a cycle of length 4; By Lemma 8, any three cycles have a common vertex v_0 ; By Lemma 10, any tree attaches to the same vertex u . Now we show that $u = v_0$. Otherwise, if $u \neq v_0$ and $d(v_0) \geq d(u)$, let C^* be the cycle that contains u and $G' = (G - \{uy | y \in N(u) - V(C^*)\}) \cup \{v_0 y | y \in N(u) - V(C^*)\}$ with $|N(u) - V(C^*)| = t_1$, by Fact 2 and $d_{G'}(u) = d(u) - t_1, d_{G'}(v_0) = d(v_0) + t_1$, we have

$$\frac{\Pi_2(G)}{\Pi_2(G')} = \frac{d(v_0)^{d(v_0)} d(u)^{d(u)}}{[d(v_0) + t_1]^{d(v_0)+t_1} [d(u) - t_1]^{d(u)-t_1}} = \frac{\frac{d(v_0)^{d(v_0)}}{[d(v_0)+t_1]^{d(v_0)+t_1}}}{\frac{[d(u)-t_1]^{d(u)-t_1}}{d(u)^{d(u)}}} < 1,$$

that is, $\Pi_2(G') > \Pi_2(G)$, a contradiction with the choice of G ; If $d(u) > d(v_0)$, let $G'' = (G - \{v_0 y | y \in N(v_0) - V(C^*)\}) \cup \{uy | y \in N(v_0) - V(C^*)\}$ with $|N(u) - V(C^*)| = t_2$, by Fact 2 and

$d_{G''}(v_0) = d(v_0) - t_2$, $d_{G''}(u) = d(u) + t_2$, we have

$$\frac{\Pi_2(G)}{\Pi_2(G'')} = \frac{d(u)^{d(u)} d(v_0)^{d(v_0)}}{[d(u) + t_2]^{d(u)+t_2} [d(v_0) - t_2]^{d(v_0)-t_2}} = \frac{\frac{d(u)^{d(u)}}{[d(u)+t_2]^{d(u)+t_2}}}{\frac{[d(v_0)-t_2]^{d(v_0)-t_2}}{d(v_0)^{d(v_0)}}} < 1,$$

that is, $\Pi_2(G'') > \Pi_2(G)$, a contradiction with the choice of G . Therefore, we can obtain the construction of G as follows: If $n - k \equiv 0 \pmod{2}$, then the degree sequence of G is $n - 2, \underbrace{2, 2, \dots, 2}_{n-k-1}, \underbrace{1, 1, \dots, 1}_k$; if $n - k \equiv 1 \pmod{2}$, then the degree sequence of G is $n - 1, \underbrace{2, 2, \dots, 2}_{n-k-1}, \underbrace{1, 1, \dots, 1}_k$. Thus, Theorem 5 is true. \square

4 Compliance with Ethical Standards

Conflict of interest: Shaohui Wang and Bing Wei state that there are no conflicts of interest. Patients rights and animal protection statements: This article does not contain any studies with human or animal subjects.

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